



Accurate Mass: 234.050379
Percentage Composition: C 51.29%; H 3.87%; F 24.34%; O 20.50%
Optical Rotation: $[\alpha]_D +6.9$ (neat)
Other Data: Not opt. pure

>> **Derivative:** Me ether

CAS Registry Number: 17257-71-5

Use/Importance: Reagent for detn. of optical purity of alcohols and amines
Melting Point: Mp 43-45°. Mp 46-49°
Boiling Point: Bp_{0.05} 95-97°. Bp_{1.5} 115-117°
Optical Rotation: $[\alpha]_D -71.8$ (c, 3.28 in MeOH)
Aldrich: 15561-6
Fluka: 65364
Sigma: M9385

>> **Variant:** (±)-form

CAS Registry Number: 395-35-7
Molecular Formula: C₉H₇F₃O₃
Molecular Weight: 220.148
Accurate Mass: 220.034729
Percentage Composition: C 49.10%; H 3.20%; F 25.89%; O 21.80%
Physical Description: Cryst (C₆H₆)
Melting Point: Mp 110.5-111.5°
Aldrich: 23307-2

>> **Derivative:** Me ester

Boiling Point: Bp_{2.5} 86-92° (lit. gives a pressure range)

>> **Derivative:** Amide

Molecular Formula: C₉H₈F₃NO₂
Molecular Weight: 219.163
Accurate Mass: 219.050713
Percentage Composition: C 49.32%; H 3.68%; F 26.01%; N 6.39%; O 14.60%
Physical Description: Cryst. (C₆H₆/hexane)
Melting Point: Mp 102-103°

>> **Derivative:** Nitrile

Synonym(s): 1-Cyano-2,2,2-trifluoro-1-phenylethanol. 2,2,2-Trifluoroacetophenone cyanohydrin

Molecular Formula: C₉H₆F₃NO
Molecular Weight: 201.148
Accurate Mass: 201.040148
Percentage Composition: C 53.74%; H 3.01%; F 28.33%; N 6.96%; O 7.95%
Physical Description: Cryst. (hexane)
Melting Point: Mp 75-77°

>> **Derivative:** Me ether

CAS Registry Number: 56135-03-6
Use/Importance: Nmr shift reagent
Melting Point: Mp 44-45°
Boiling Point: Bp₁ 105-110°
Aldrich: 15655-8

References: